7-24-2018

Novel high-performance ingredients based on functionalized polysaccharides – The role of enzymatic catalysis.

Stefan Ulvenlund
Enza Biotech, AB, Sweden, stefan.ulvenlund@enzabiotech.com

Novel High-Performance Ingredients Based on Functionalized Polysaccharides. The Role of Enzymatic Catalysis.

ECI Advances in Cosmetic Formulation Design

July 24, 2018

Stefan Ulvenlund

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Biotechnology for a green future

Enza Biotech AB founded in 2012
Spin-off from Lund University, Sweden
Acquired by Croda International Plc in July 2017

Enza is now acting as the Croda Centre of Innovation in Carbohydrate Chemistry

Why Carbohydrates?

We all know that they are

- Green and sustainable
- Biodegradable
- Generally non-toxic

But they are also

- Chemically stable
- Highly *functional*
  - Introducing ”green” ingredients is a way to introduce *new* functionalities
- *Efficient* ingredients
  - More efficient ingredients translate as less material and potentially lower cost

Sugar – you can’t beet it!

Cost – Efficiency – Consumer Preferences

- *”Everybody wants to save the planet, but nobody wants to pay for it”*
- It is often, erroneously, assumed that the price per unit mass of green materials has to be the same, or lower, than that of conventional petrochemical materials
- …which would be very difficult, or indeed impossible, to achieve

vs

Cost *versus* Efficiency

AMOUNT
required

YESTERDAY
Petrochemistry

TODAY
Green+petro

COST
per unit mass

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Cost *versus* Efficiency

AMOUNT
required

YESTERDAY
Petrochemistry

TODAY
Green+petro

TOMORROW

COST
per unit mass

Cost *versus* Efficiency

AMOUNT
required

YESTERDAY
Petrochemistry

TODAY
Green+petro

TOMORROW
Green

Molecular <u>design</u>
and
optimisation for
performance

COST
per unit mass

Cost – Efficiency – *Consumer Perception - Functionality*

Cost
Decreasing price per unit mass

Efficiency
Decreasing amount of material

Customer perception
Increasing "greenness"

Functionality
New ways to formulate

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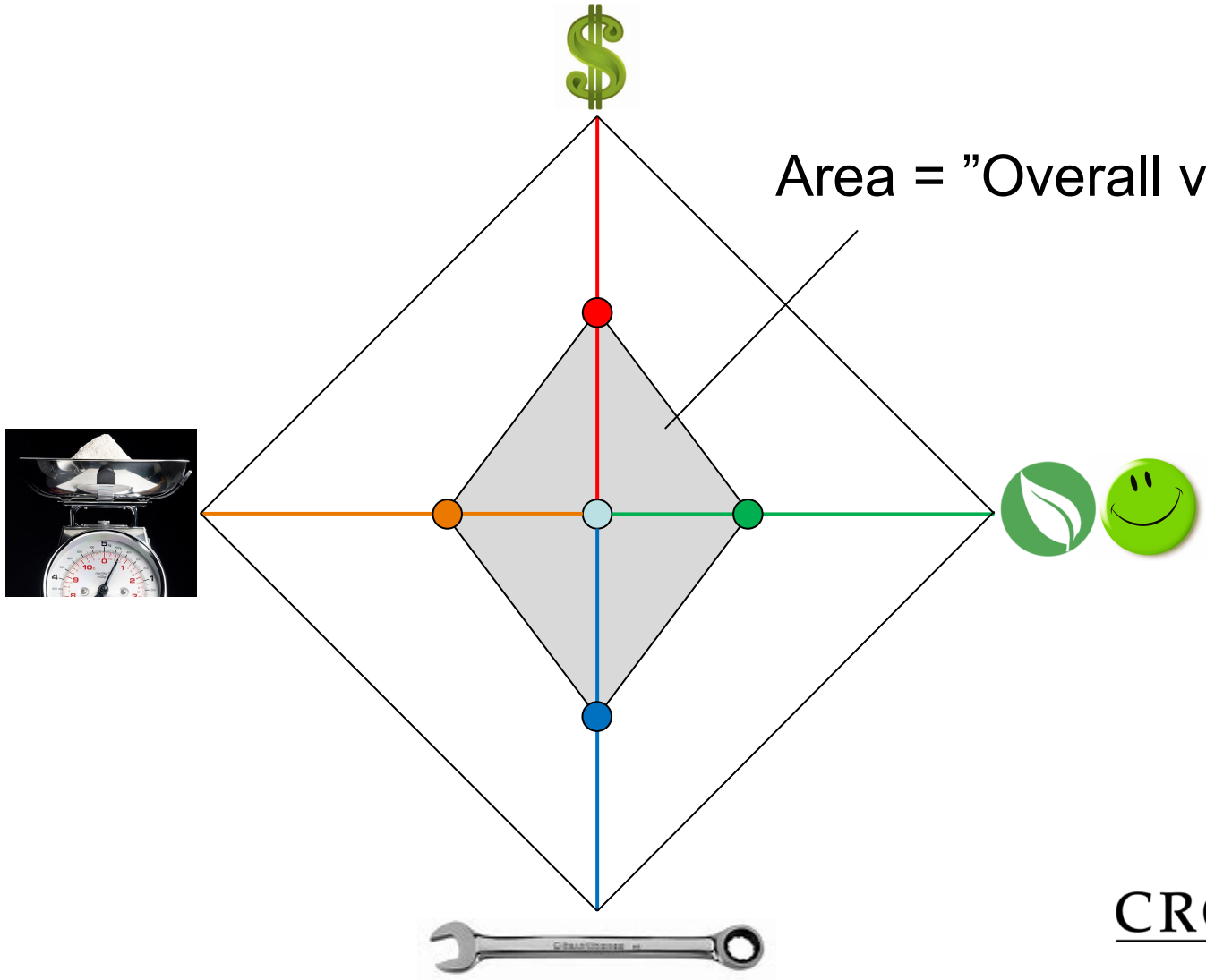
Cost – Efficiency – *Consumer Perception - Functionality*



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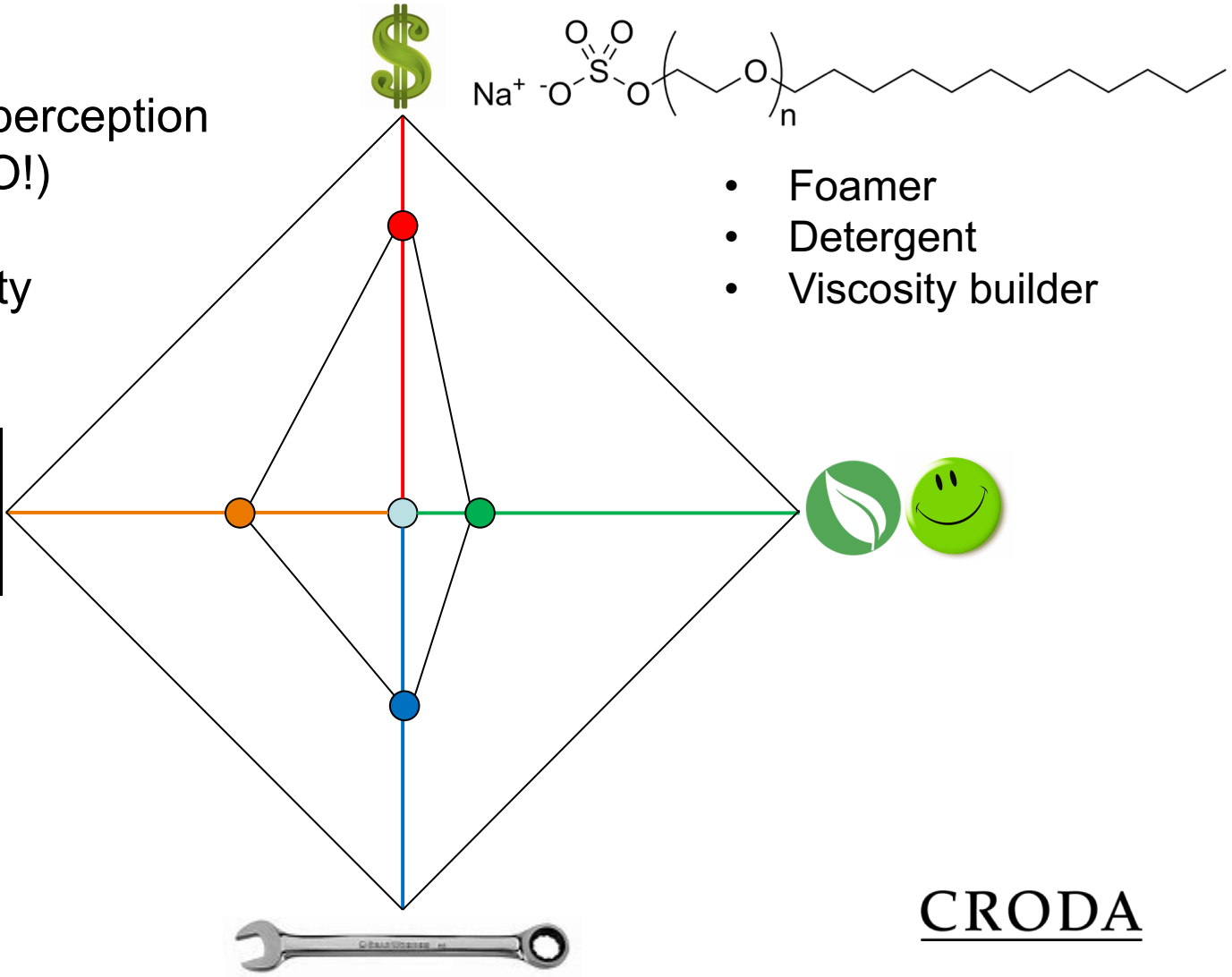
Cost – Efficiency – *Consumer Perception - Functionality*

Example: SLES

- Poor consumer perception (sulphate *and* EO!)
- Dirt cheap
- Good functionality
- Very efficient



- Foamer
- Detergent
- Viscosity builder

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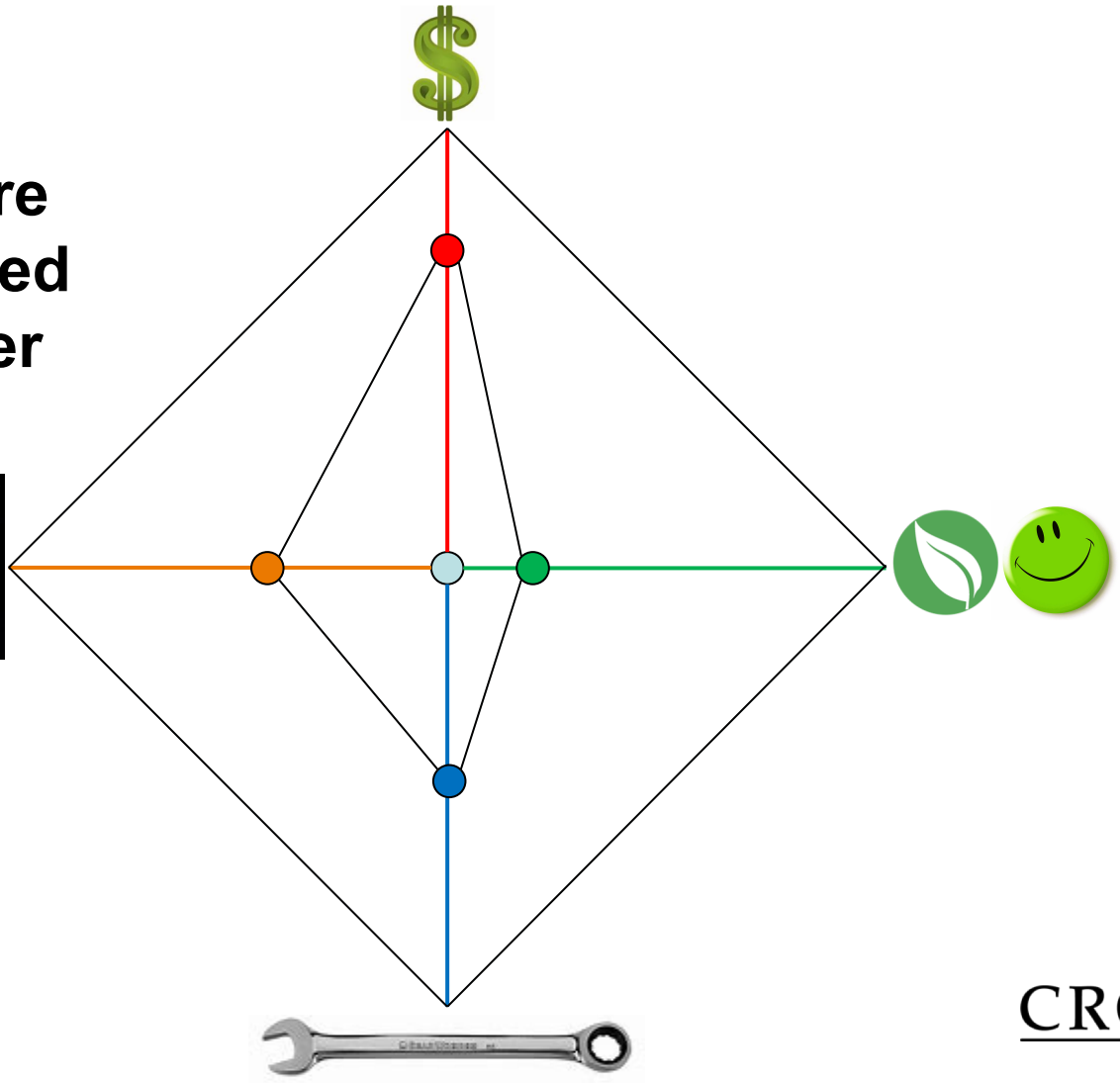
Cost – Efficiency – *Consumer Perception - Functionality*

Cost **and**
efficiency **are directly linked to each other**



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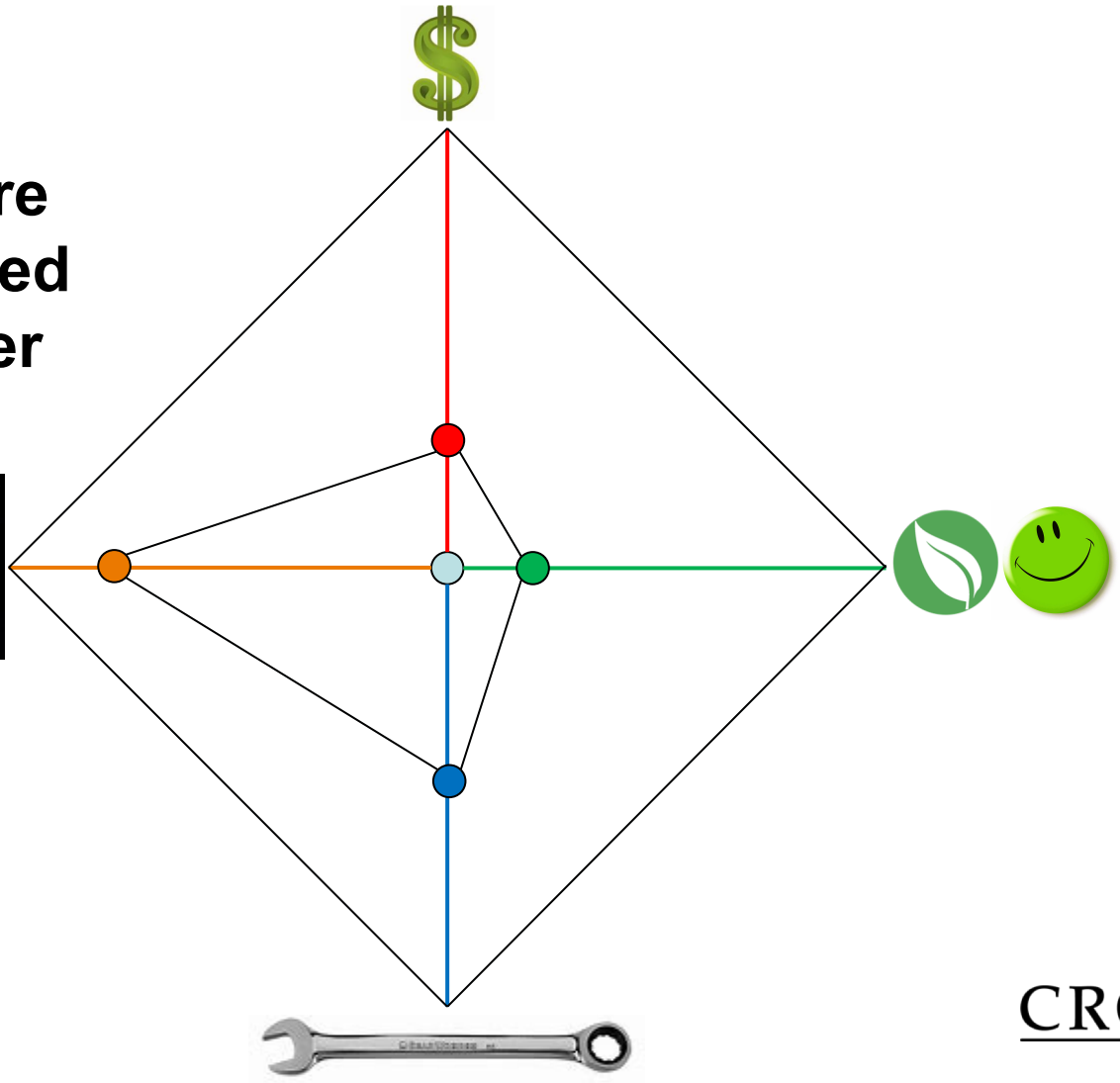

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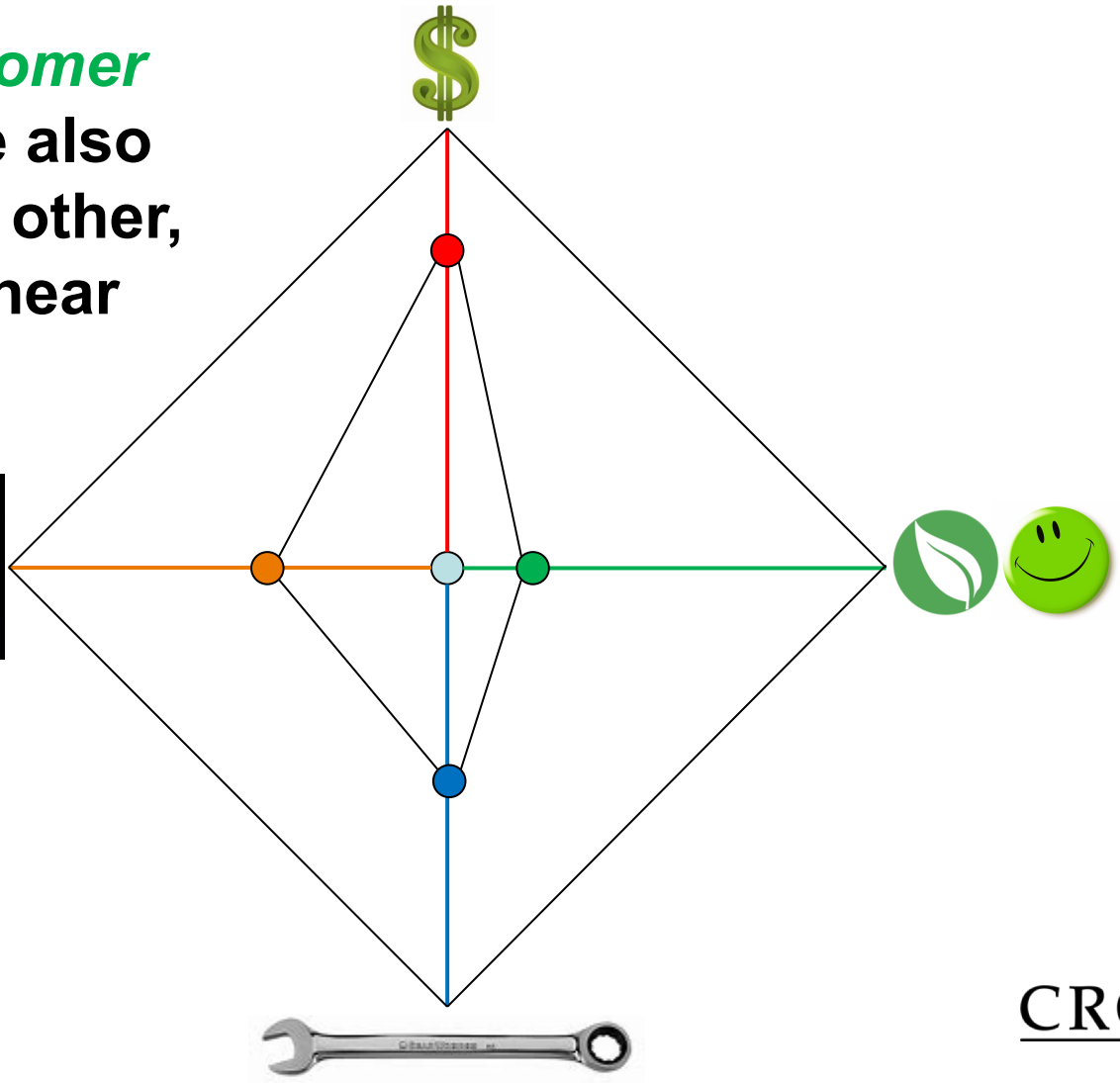
Cost – Efficiency – *Consumer Perception - Functionality*

Cost **and** ***customer perception*** **are also linked to each other, but in a non-linear way**



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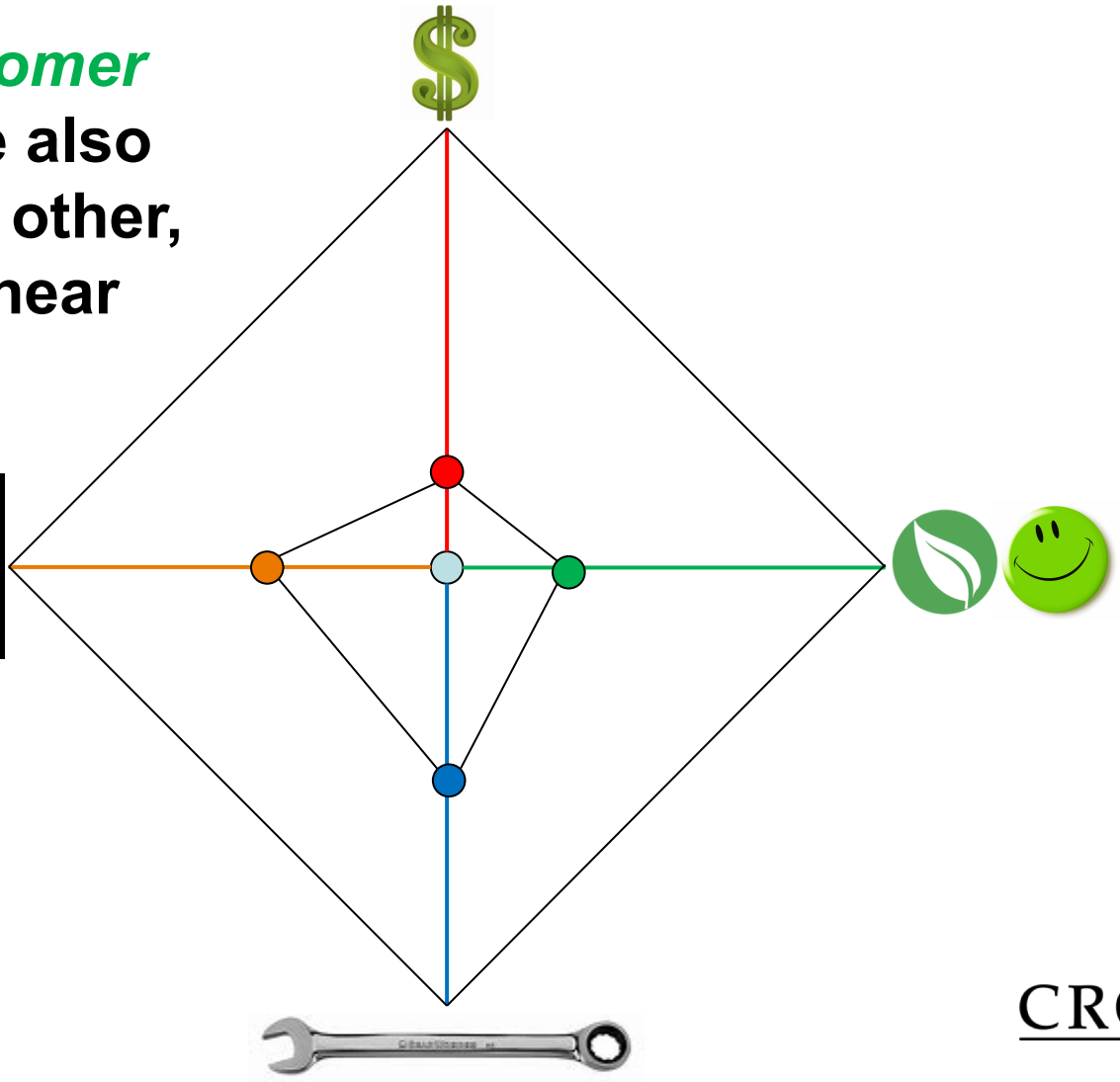

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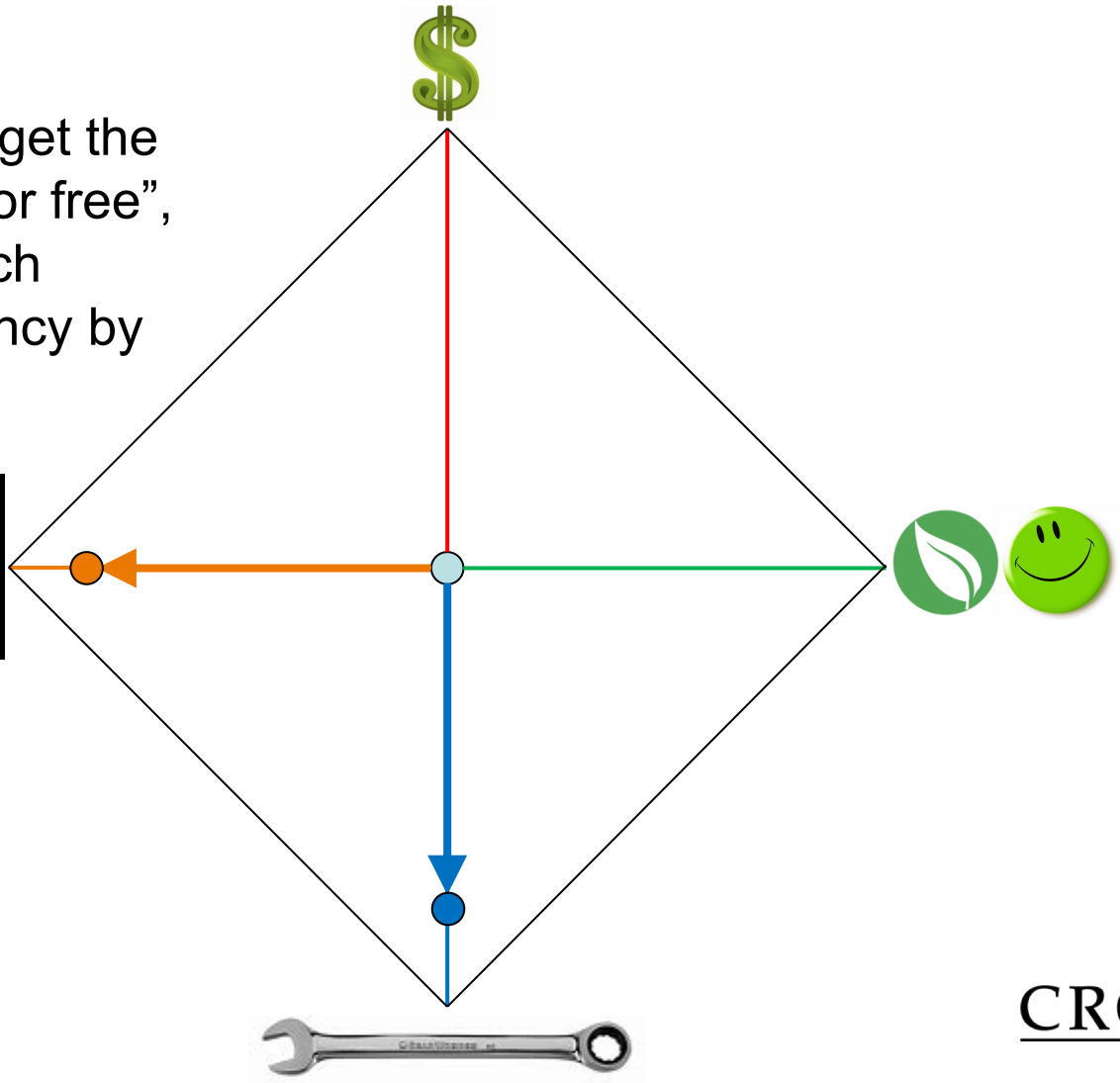
Cost – Efficiency – *Consumer Perception - Functionality*

When working with carbohydrates, we get the ”green dimension for free”, but we can approach function and efficiency by *rational design*



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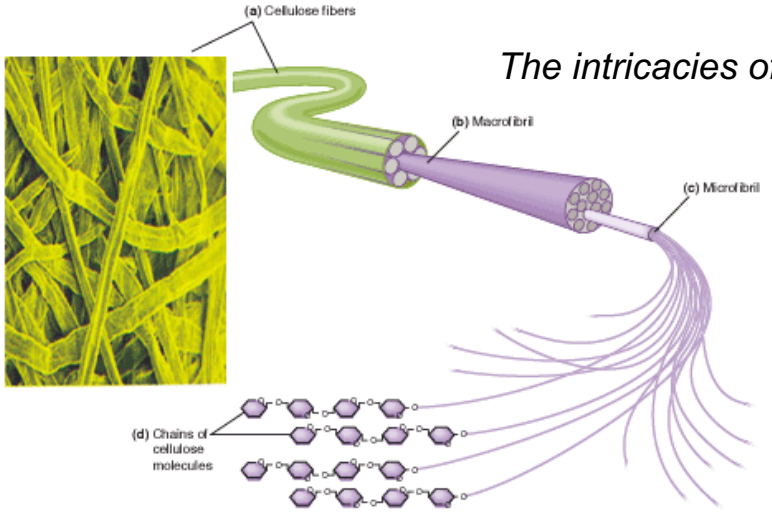
Rational Design Using Carbohydrates

- Structural complexity
  - Molecular level
  - Supramolecular level



The intricacies of cellulose

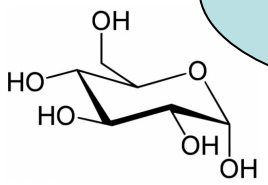
- If we understand the structure-function relationship, we can use it to our advantage and build
  - Efficiency
  - Function

Classification of “simple”, non-charged polysaccharides*

STARCH

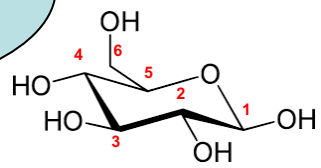
- Dextran — α-1,6
- Amylose — α-1,4
- Amylo-pectin — α-1,4+ α-1,6
- Pullulan — α-1,6

α



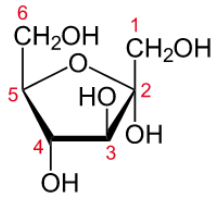
Glucans

β



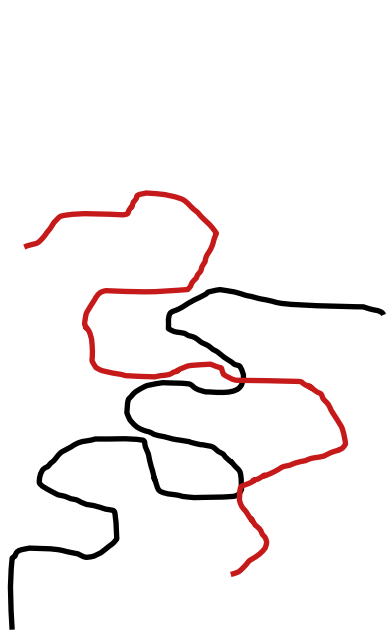
- β-1,4 — Cellulose — Insoluble
- β-1,3 — Curdlan
- β-1,3 — Sclerotium
- β-1,3+ β-1,4 — Oat glucan

- Levan — β-2,6 — High-MW. Used in cosmetics, but not as thickener
- **Fructans**
- Inulin — β-2,1 — Low-MW. Used in cosmetics as humeactant.

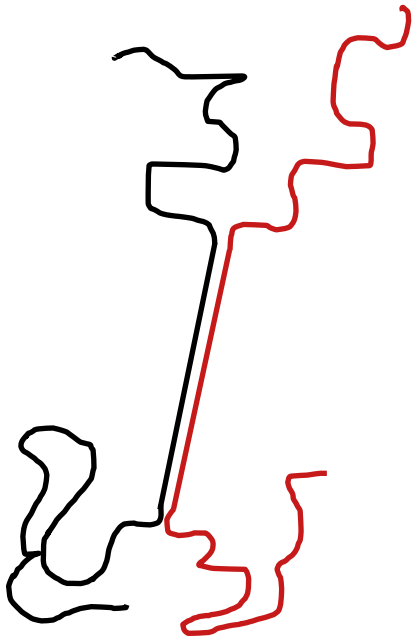


* “Simple” refers to chemical composition only

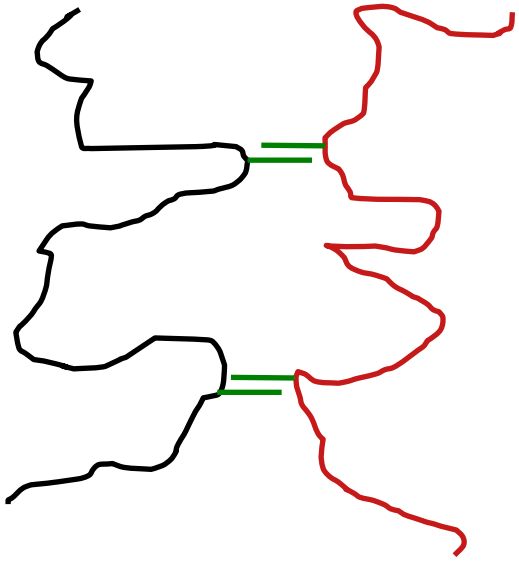
Modes of self-association in aqueous polysaccharide systems



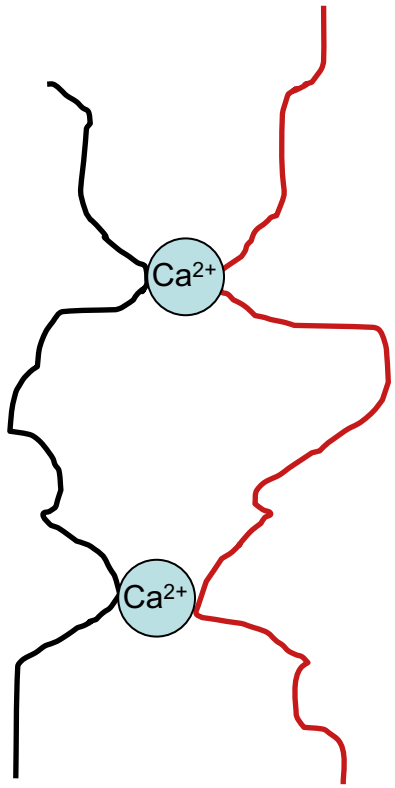
Entanglement



Helix formation and/or H-bonds

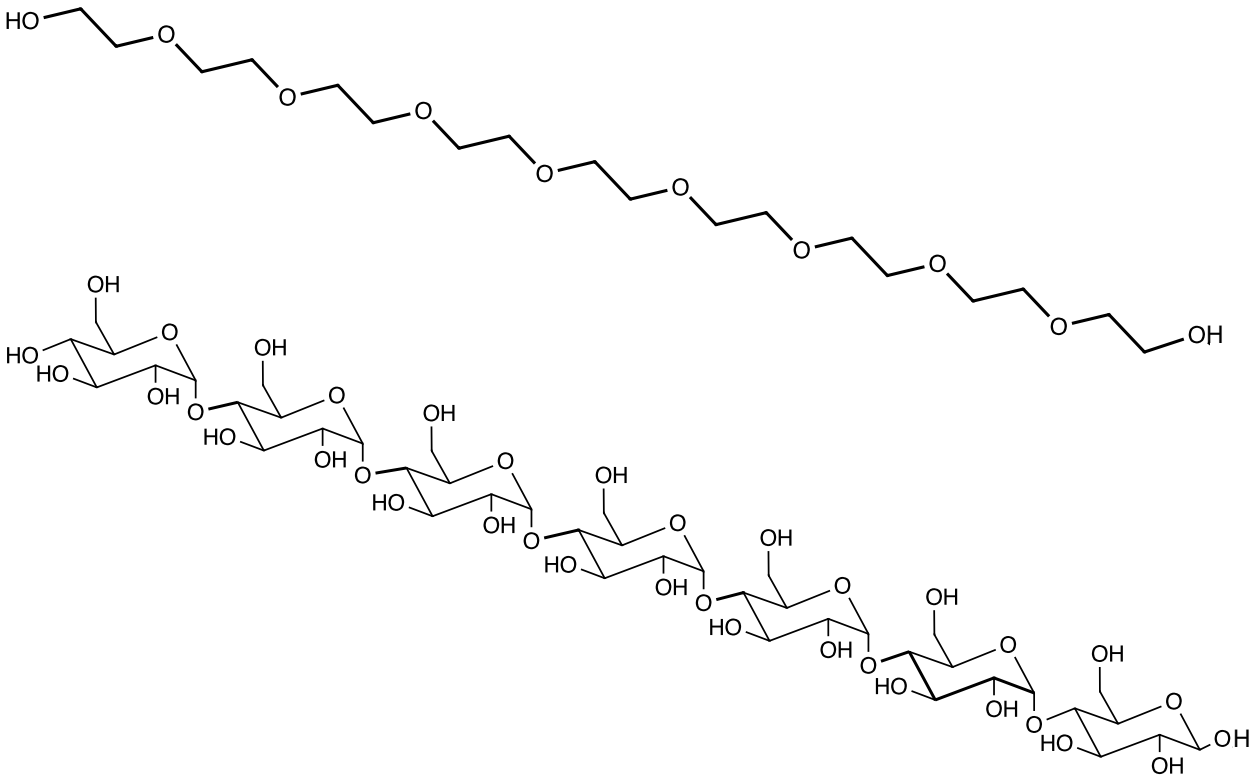


Hydrophobic interactions



Ionic interaction

Molecular Architecture



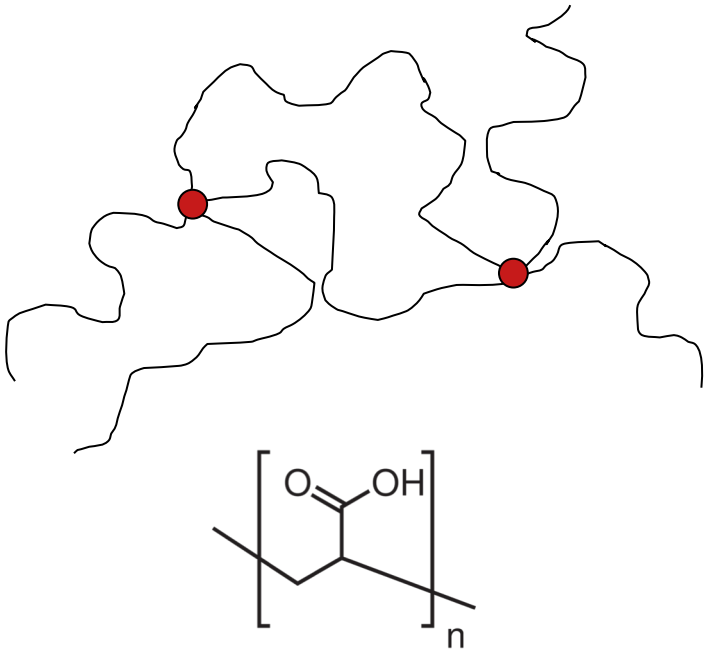
Polyethyleneglycol (PEG)

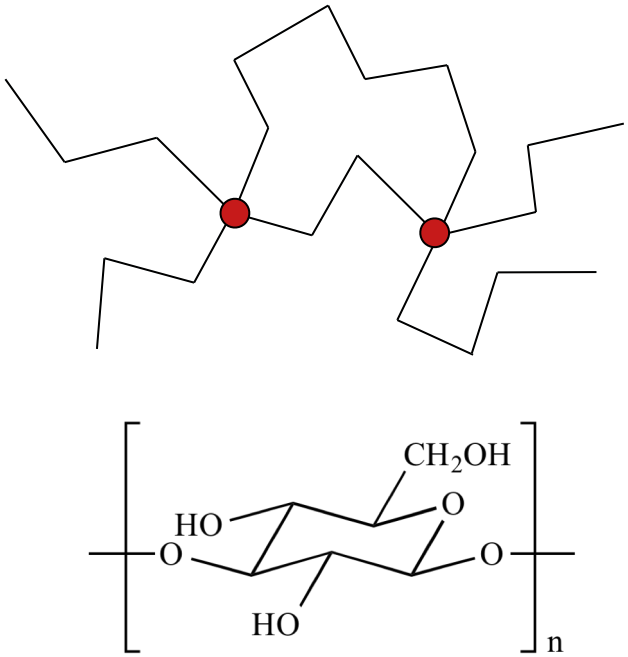
- Freely jointed head-group chain
- Small excluded volume
- Limited hydration
- No self-association

Amylose

- Rigid subunits
- Large excluded volume
- Extensive hydration
- Molecular and supramolecular complexity
- Self-association

Rigidity Impacts Performance





Carbomers (”Super-slurps”)

Freely jointed chains

Extremely efficient swelling

Cross-linked carbohydrates

Rigid subunits

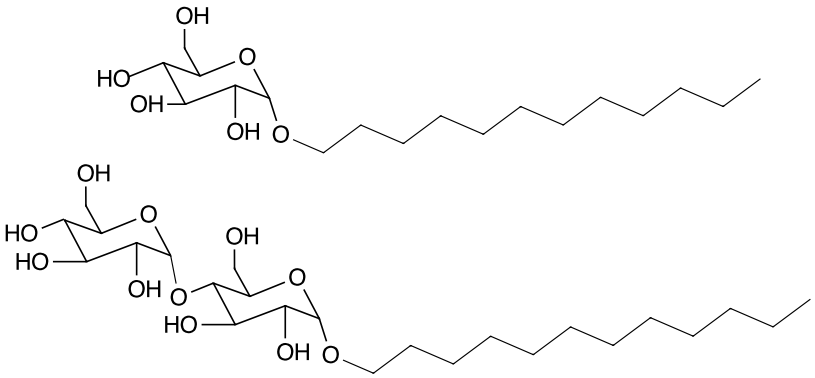
Restricted swelling

Why Enzymes?

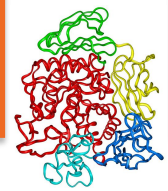
- Compatible with The Principles of Green Chemistry
  - Low temperatures
  - Water as solvent
  - Derived from ”natural” sources
  - Biodegradable and non-toxic
- There are 1000s of enzymes designed by Nature and improved by Man that act on carbohydrates
- Many of these enzymes are available in bulk quantities
  - Amylases (food and feed)
  - Cellulases (laundry)
  - Pullullanases (grain processing)
  - …etc

Enzymes at Work:
Elongation of Alkylglycoside Surfactants

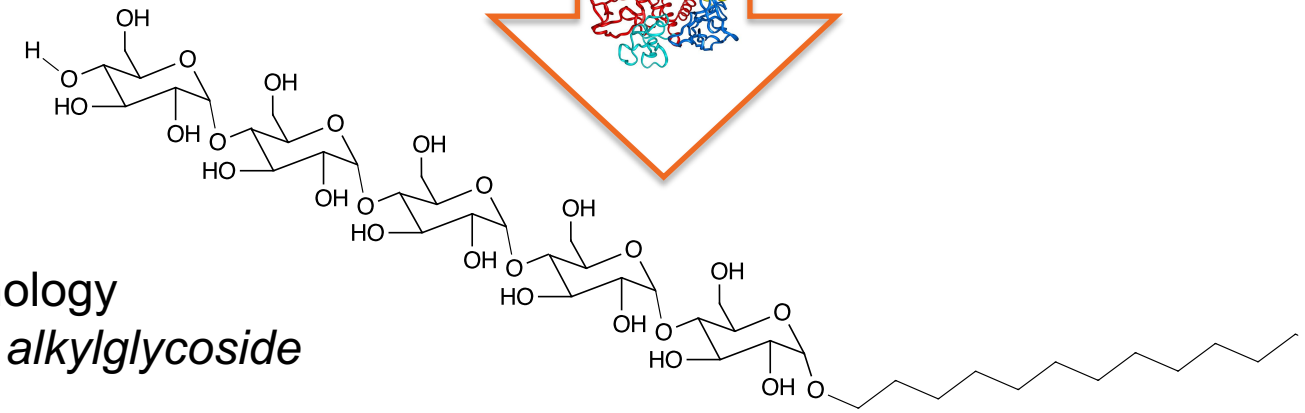
Conventional technology
"Alkylpolyglycosides"- APG



+ CGTase



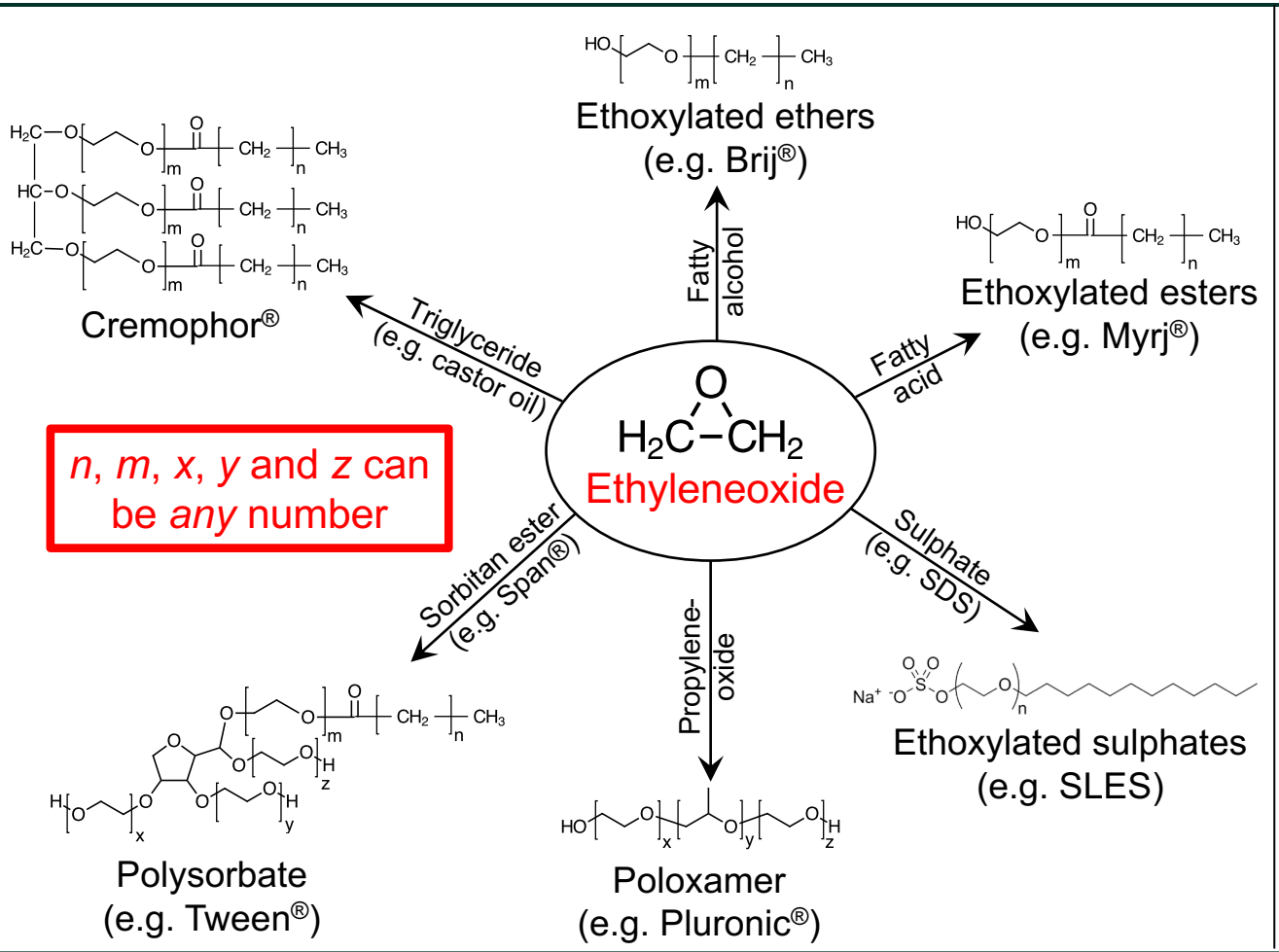
+ Glucose donor

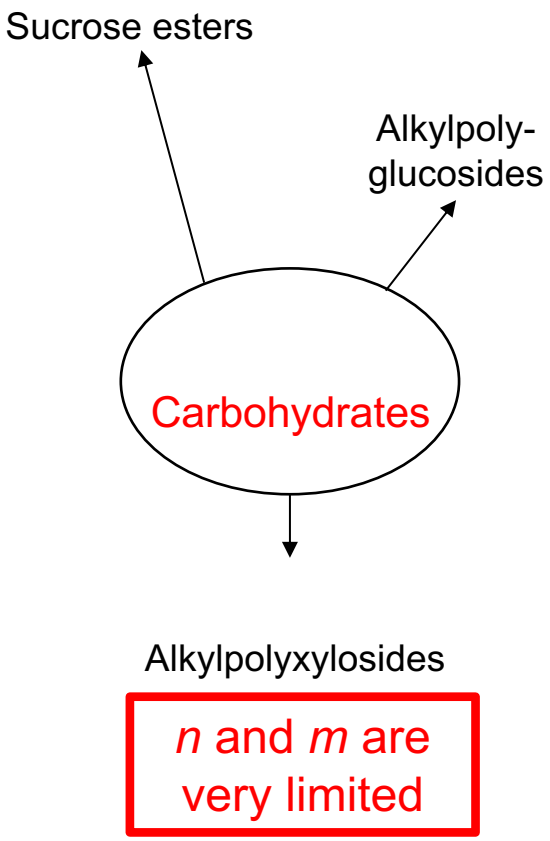


Enza technology
Oligomeric alkylglycoside

Versatility

To Do With Sugar What We Already Do with Ethoxylates

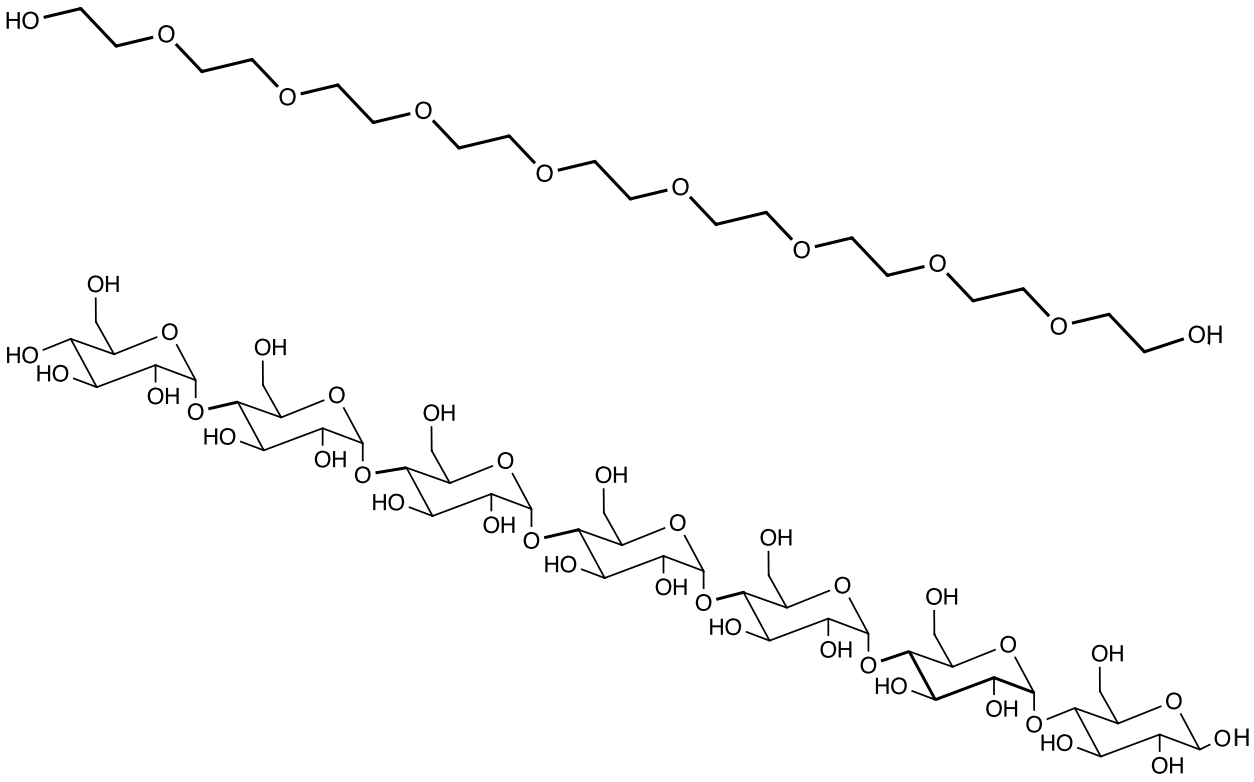




Other Reasons to Elongate Alkylglycosides

- Toxicity and irritancy
  - Increasing head-group length decreases cell toxicity
- Solubility
  - Making it possible to create surfactants with >12 C that are soluble at room temperarture
- Efficiency and functionality
  - This is *not* about mimicing the performance of ethoxylates, or about replacing them
  - This is about finding new applications and enabling novel types of formulations

Molecular Architecture



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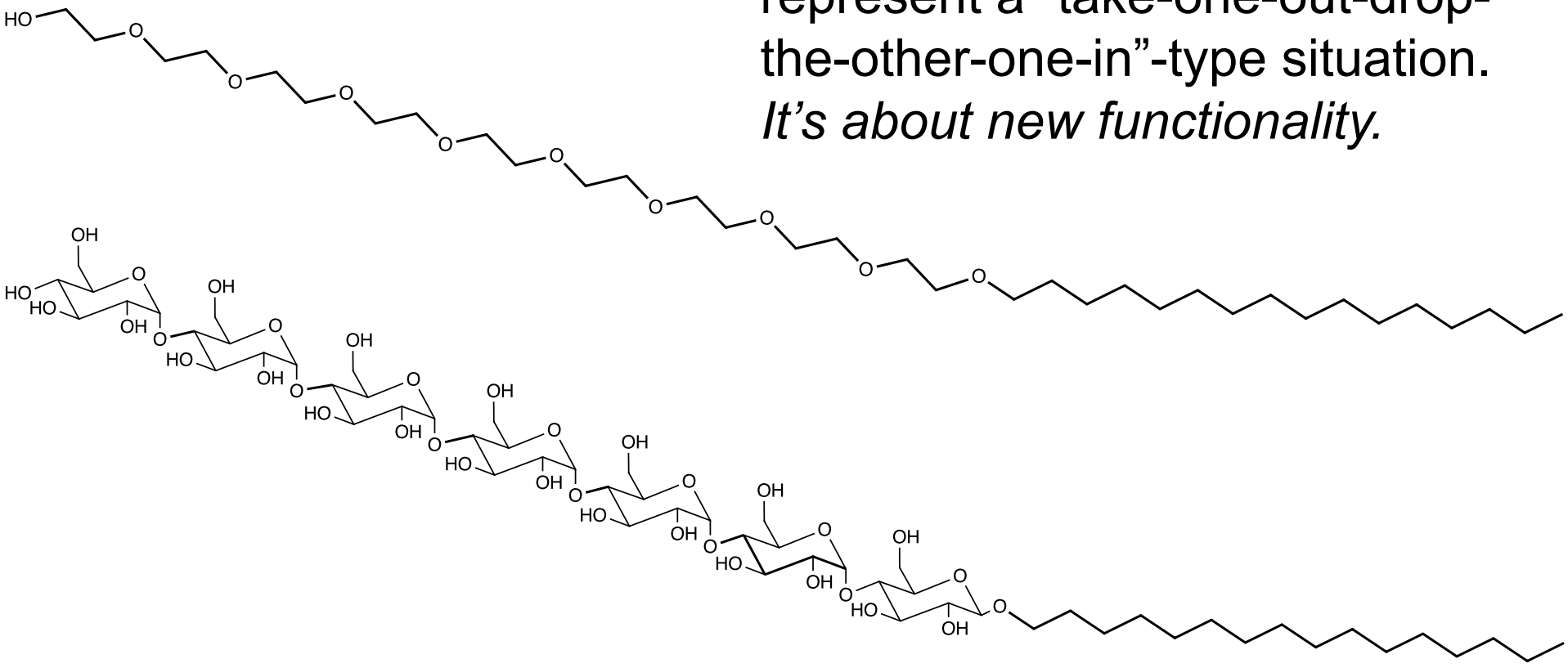
- Freely jointed head-group chain
- Small excluded volume
- Limited hydration
- No self-association

Amylose

- Rigid subunits
- Large excluded volume
- Extensive hydration
- Molecular and supramolecular complexity
- Self-association

Molecular Architecture

These surfactants do not represent a ”take-one-out-drop-the-other-one-in”-type situation. *It’s about new functionality.*



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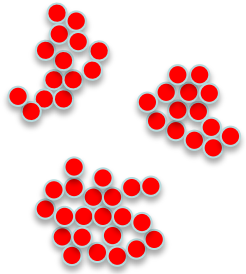
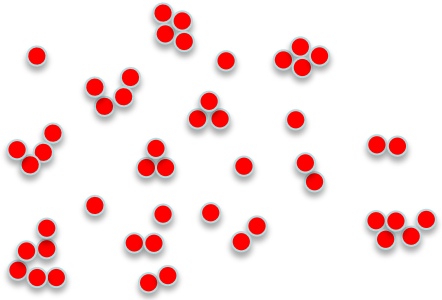
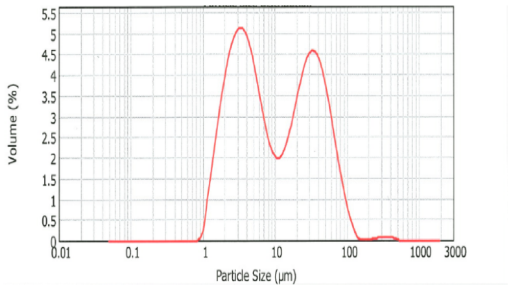
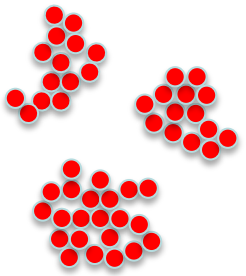
Wetting and dispersion of hydrophobic particles



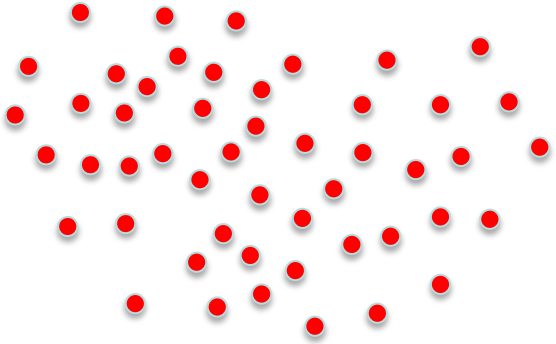
Poor wetting agent

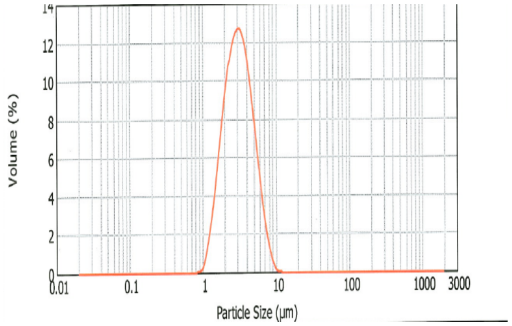






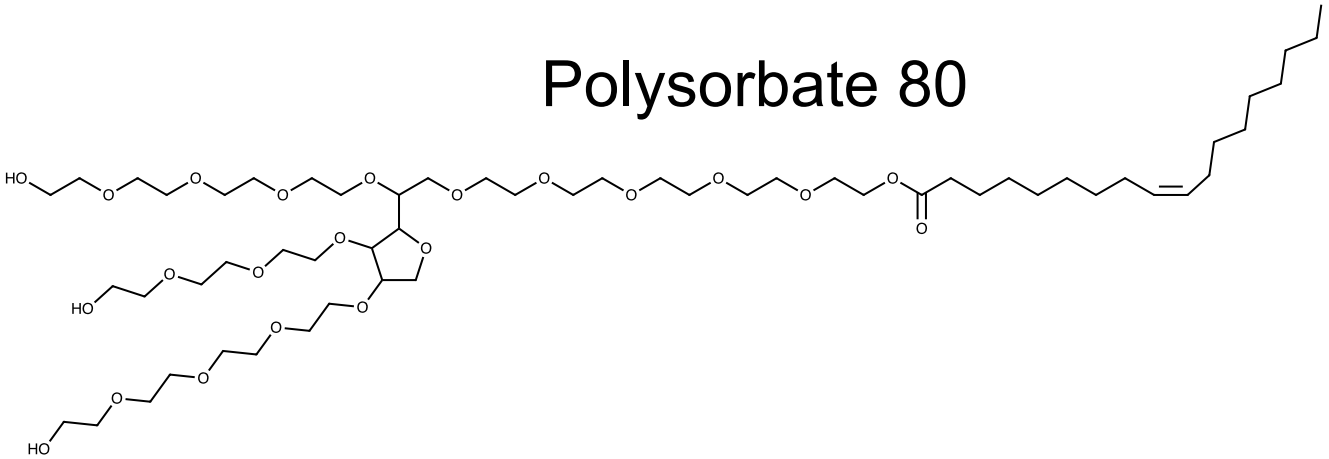
Good wetting agent

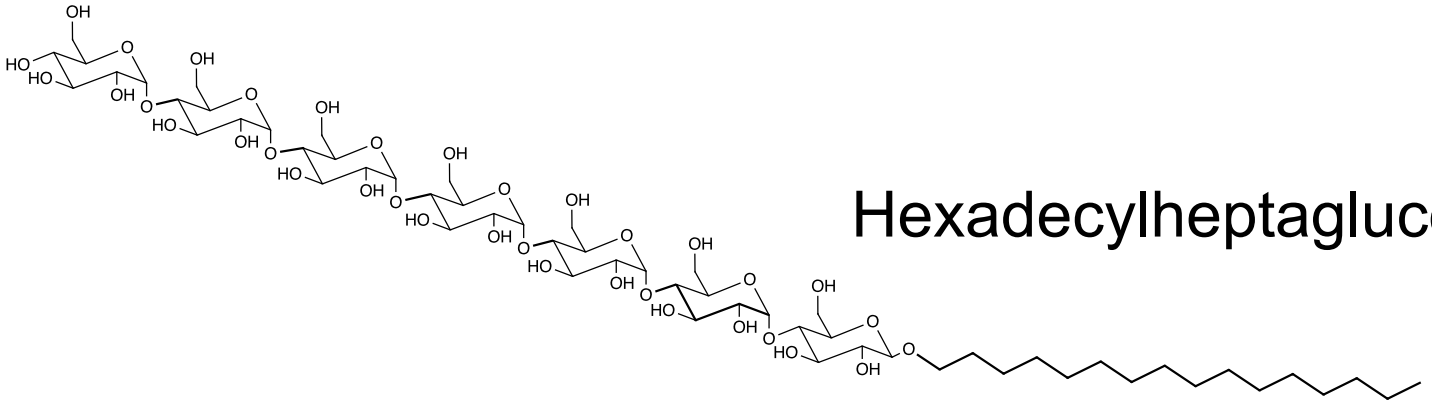




The Contenders

Polysorbate 80

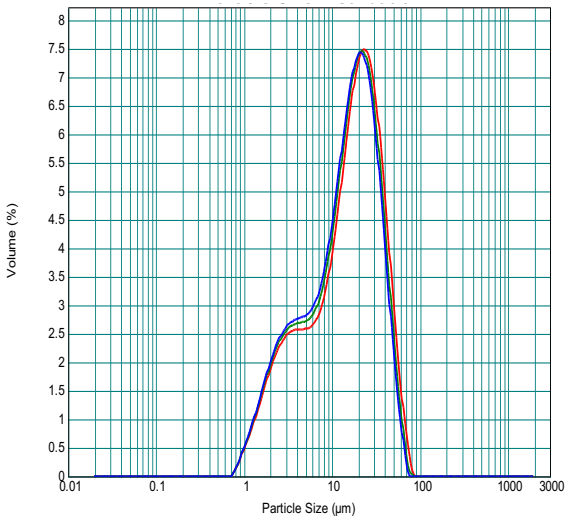




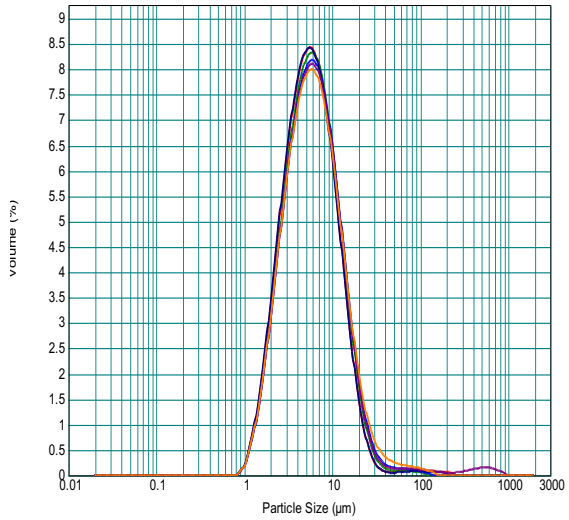
Hexadecylheptaglucoside ($C_{16}G_7$)

Wetting of micronized BDP under low-shear conditions

Polysorbate 80
standard grade



Enza
$C_{16}G_7$



Data on micronised beclomethasone dipropionate

In Conclusion

- Think function
- Think efficiency
- Think rational design, based on structure-function relationships
- Use what's already our there as a starting point
  - Enzymes
  - Starting materials
- *The is a lot out there*

In 2015, the Cosmetic Ingredient Review Expert Panel (Washington) reviewed the safety of 106 polysaccharides that are used as thickeners in cosmetic products

Safety Assessment of
Polysaccharide Gums as Used in Cosmetics

Status:	Final Report
Release Date:	October 22, 2015
Panel Date:	September 21-22, 2015

Available for download at http://www.cir-safety.org/sites/default/files/plpogu092015final.pdf